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Exact Calculation of the Second-Order Born Terms for Proton-Hydrogen Electron-Transfer Collisions*

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The four second-order terms in the Born series for the proton-hydrogen electron-transfer problem are analytically reduced from six-dimensional to three-dimensional integrals. No mass approximations are made. This permits an accurate numerical calculation of the total cross section to second order. Numerical results are given from 0.1 to 2.5 MeV. The complete second-order cross section reduces the first-order results by 30% from 1 to 2.5 MeV. The various first- and second-order Born approximations for this problem are discussed.

I. INTRODUCTION

One of the most basic and widely studied three-body rearrangement processes is that of resonant proton-hydrogen electron-transfer collisions.[1] In an early classical analysis of the problem, Thomas[2] described the collision process as a two-step interaction and found that the total cross section behaved as $E^{-5.5}$ at high energy, where E is the energy of the incident proton. At about the same time, Oppenheimer[3] and Brinkman and Kramers[4] performed a quantum-mechanical calculation leading to a cross section sharply peaked in the forward direction ("pickup" process) with a high-energy behavior of E^{-6}. They used an abbreviated form of the first-order Born approximation which neglected the proton-proton interaction. This neglect is justified in the expected high-energy region of validity of the first-order Born approximation by the large proton-electron mass ratio which allows a classical description of the internuclear motion.

The neglect of the proton-proton interaction was disputed by Bates and Dalgarno[5] and by Jackson and Schiff.[6] The latter have shown that inclusion of this interaction for forward-scattering angles reduces the Brinkman–Kramers cross section at all energies and, in the high-energy limit, by a factor of 0.661. In this approximation, the energy dependence of the cross section remains as E^{-6}.

Mapleton[7] has pointed out that Jackson and Schiff erred in neglecting the contribution to the proton-proton interaction from backward-scattering angles ("knockout" process). Including this, he shows that for resonant systems at high energy the total cross section behaves as E^{-3}. However, due to the small coefficient of the E^{-3} term, the Jackson–Schiff cross section is not in error until around 50 MeV, and the E^{-3} behavior is not approached until well over 100 MeV, a region where relativistic corrections must be considered.[8] It is interesting to note that for the resonant positron-positronium system the E^{-3} behavior is readily apparent at an energy of only 200 eV.[9]

The four second-order terms of the Born approximation were first investigated by Drisko in the high-energy limit.[10] For forward-scattering angles, he found that the first-order proton-proton interaction was cancelled by some of the second-order terms. The total cross section then behaved as $E^{-5.5}$ at high energy as predicted classically by Thomas. However, he did not consider backward scattering, and his arguments need modification in that region. Also, the coefficients of the second-order terms are such that they do not dominate the first-order terms at forward-scattering angles until 50–100 MeV.

The question of the convergence of the Born series for rearrangement collisions has been raised by Aaron *et al.*[11] Their proof of nonconvergence dealt with a divergence of the Green's-

function series for rearrangement collisions, and no rigorous conclusion can be drawn about the Born series itself. Indeed, a one-dimensional counter example has been given by Dettmann and Liebfried.[12] The latter[13] have also carefully examined the asymptotic behavior of the various terms in the Born series and have concluded that for resonant systems the first-order repulsive interaction does eventually dominate the cross section because of backward scattering. At forward angles, they agree with Drisko's results. For nonresonant systems, they conclude that both the first- and second-order Born terms are needed even at high energies.

The purpose of this paper is to investigate the role of the second-order Born terms at intermediate energies (100 keV to a few MeV). In this region the various asymptotic expressions that have been used to examine the high-energy behavior are not completely valid. In Sec. II, the analytic reduction of the four second-order Born terms from six-dimensional to three-dimensional integrals is given. This permits an accurate numerical calculation of the second-order terms to be done by computer. The results are discussed in Secs. III and IV.

II. EVALUATION OF MATRIX ELEMENTS

We consider the rearrangement process in which particle 1 (proton) is incident on a bound state of particles 2 (proton) and 3 (electron):

$$1+(2,3)\rightarrow(1,3)+2 \quad . \tag{2.1}$$

After the collision, particle 2 is ejected. The first- and second-order Born-series terms for this process are, respectively,

$$T^{\mathrm{I}}_{if}=\langle\Phi_f^{(2)}\,|\,V_1+V_3\,|\,\Phi_i^{(1)}\rangle \quad , \tag{2.2a}$$

$$T^{\mathrm{II}}_{if}=\langle\Phi_f^{(2)}\,|\,V_1G_0V_2+V_1G_0V_3+V_3G_0V_2+V_3G_0V_3\,|\,\Phi_i^{(1)}\rangle \quad , \tag{2.2b}$$

where $\Phi_f^{(2)}$ represents the final three-body state with particle 2 free; $\Phi_i^{(1)}$ represents the initial three-body state with particle 1 free, V_1 is the potential between particles 2 and 3, etc.; and G_0 is the Green's function for three free particles given by

$$G_0=(S-H_0)^{-1} \quad . \tag{2.3}$$

Here S is the three-body center-of-mass energy with positive imaginary part, and H_0 is the Hamiltonian for three free particles.

The coordinate system used to evaluate the matrix elements in Eq. (2.2) describes three particles with charges Z_i, masses m_i, and momenta $\vec{\mathrm{k}}_i$ $(i=1,2,3)$. In terms of these, we define the relative momenta

$$\vec{\mathrm{k}}_{jk}=\mu_{jk}\left(\frac{\vec{\mathrm{k}}_j}{m_j}-\frac{\vec{\mathrm{k}}_k}{m_k}\right) \quad , \tag{2.4}$$

$$\vec{\mathrm{p}}_i=\mu_i\left(\frac{\vec{\mathrm{k}}_j+\vec{\mathrm{k}}_k}{m_j+m_k}\right)-\frac{\mu_i\vec{\mathrm{k}}_i}{m_i} \quad (i,j,k \text{ cyclic}) \quad , \tag{2.5}$$

where

$$\mu_i=\frac{m_i(m_j+m_k)}{m_i+m_j+m_k} \quad \text{and} \quad \mu_{jk}=\frac{m_jm_k}{m_j+m_k} \quad . \tag{2.6}$$

The three sets of $\vec{\mathrm{p}}_i$, $\vec{\mathrm{k}}_{jk}$ are related by

$$\vec{\mathrm{p}}_i=-(\mu_{ki}/m_k)\vec{\mathrm{p}}_j+\vec{\mathrm{k}}_{ki} \quad , \tag{2.7}$$

$$\vec{\mathrm{k}}_{jk}=-(\mu_{jk}/\mu_j)\vec{\mathrm{p}}_j-(\mu_{jk}/m_k)\vec{\mathrm{k}}_{ki} \quad (i,j,k \text{ cyclic}) \quad . \tag{2.8}$$

In this coordinate system, the matrix element for the process [Eq. (2.1)] can be written

$$\langle\Phi_f^{(2)}\,|\,M\,|\,\Phi_i^{(1)}\rangle=64\pi\lambda^5\int\frac{d\vec{\mathrm{k}}_{31}}{(\lambda^2+k_{31}^2)^2}\int\frac{d\vec{\mathrm{k}}_{23}}{(\lambda^2+k_{23}^2)^2}\times\langle\vec{\mathrm{p}}_2'\vec{\mathrm{k}}_{31}\,|\,M\,|\,\vec{\mathrm{p}}_1'\vec{\mathrm{k}}_{23}\rangle \quad , \tag{2.9}$$

where $\vec{\mathrm{p}}_1'$ and $\vec{\mathrm{p}}_2'$ are the initial and final momenta, respectively, for the free proton (with the scattering angle θ given by $\hat{p}_1'\cdot\hat{p}_2'=-\cos\theta$); M is any of the operators in Eq. (2.2); and where the two-body bound states in Eq. (2.1) were taken to be the ground state of hydrogen with $\lambda=\mu_{23}e^2=a_0^{-1}$ as the reciprocal Bohr radius. The differential cross section to second order in the Born series is given by

$$\frac{d\sigma}{d\Omega}=\frac{\mu_1\mu_2}{(2\pi)^2}\frac{|\vec{\mathrm{p}}_2'|}{|\vec{\mathrm{p}}_1'|}\,|T^{\mathrm{I}}_{if}+T^{\mathrm{II}}_{if}|^2 \quad . \tag{2.10}$$

A. First-Order Terms

The first-order terms have been extensively referred to in the literature and are given for reference in the present notation. Using the Coulomb potential

$$\langle\vec{\mathrm{p}}_i\vec{\mathrm{k}}_{jk}\,|\,V_i\,|\,\vec{\mathrm{p}}_i'\vec{\mathrm{k}}_{jk}'\rangle=\frac{\delta(\vec{\mathrm{p}}_i-\vec{\mathrm{p}}_i')Z_kZ_je^4}{2\pi^2|\vec{\mathrm{k}}_{jk}-\vec{\mathrm{k}}_{jk}'|^2} \quad , \tag{2.11}$$

the matrix element evaluated by Brinkman and Kramers is

$$\langle\Phi_f^{(2)}\,|\,V_1\,|\,\Phi_i^{(1)}\rangle=-32\pi\lambda^4e^2/(\lambda^2+A^2)^3 \quad , \tag{2.12}$$

where

$$\vec{\mathrm{A}}=\vec{\mathrm{p}}_1'+(\mu_{31}/m_3)\vec{\mathrm{p}}_2' \quad . \tag{2.13}$$

To first order in the electron-proton mass ratio, Eq. (2.12) leads to the cross section[6] (in units of a_0^2)

$$\sigma_{\mathrm{BK}}=40.2/E(1+E)^5 \quad , \tag{2.14}$$

where E is the proton energy in the lab system in units of 100 keV.

The matrix element of V_3 has been evaluated by Jackson and Schiff and may be written as[9]

$$\langle\Phi_f^{(2)}|V_3|\Phi_i^{(1)}\rangle=\frac{-\langle\Phi_f^{(2)}|V_1|\Phi_i^{(1)}\rangle}{2(B^2-\vec{B}\cdot\vec{A})}\left[\frac{(3B^2-\vec{B}\cdot\vec{A})\lambda}{(2B^2-2\vec{B}\cdot\vec{A})^{1/2}}\tan^{-1}\left(\frac{B^2-\vec{B}\cdot\vec{A}}{2\lambda^2}\right)^{1/2}\right.$$
$$\left.+\frac{B^2(B^4+B^2\lambda^2-\lambda^4)+\vec{B}\cdot\vec{A}(\lambda^2(\vec{B}\cdot\vec{A}-2\lambda^2)-(B^2+\lambda^2)^2}{(B^2-\vec{B}\cdot\vec{A}+2\lambda^2)^2}\right], \quad (2.15)$$

where

$$\vec{B}=\vec{p}_1'\,\mu_{23}/m_3+\vec{p}_2'. \quad (2.16)$$

In deriving Eqs. (2.12) and (2.15), $m_1=m_2$ was used, but no approximations were made.

In evaluating Eq. (2.15) for the scattering angle $\theta=180°$, a limit must be taken. The limiting form is

$$\langle\Phi_f^{(2)}|V_3|\Phi_i^{(1)}\rangle=(-\langle\Phi_f^{(2)}|V_1|\Phi_i^{(1)}\rangle/24\lambda^4)$$
$$\times(15\lambda^4+10\lambda^2B^2+3B^4)\quad(\theta=180°\text{ only}). \quad (2.17)$$

Neglecting backward scattering and keeping only the leading energy dependence, Jackson and Schiff have given an analytic formula for the first-order total cross section σ_{JS}.[6]

B. Second-Order Terms

The first of the four second-order matrix elements from Eqs. (2.2b) and (2.9) is

$$\langle\Phi_f^{(2)}|V_1G_0V_2|\Phi_i^{(1)}\rangle=64\pi\lambda^5\int\frac{d\vec{k}_{31}}{(\lambda^2+k_{31}^2)^2}\int\frac{d\vec{k}_{23}}{(\lambda^2+k_{23}^2)^2}$$
$$\times\langle\vec{p}_2'\vec{k}_{31}|V_1G_0V_2|\vec{p}_1'\vec{k}_{23}\rangle. \quad (2.18)$$

The integrand can be expanded by introducing the complete set of basis vectors $|\vec{p}_2''\vec{k}_{31}''\rangle$:

$$\langle\vec{p}_2'\vec{k}_{31}|V_1G_0V_2|\vec{p}_1'\vec{k}_{23}\rangle$$
$$=\int d\vec{p}_2''\int d\vec{k}_{31}''\frac{\langle\vec{p}_2'\vec{k}_{31}|V_1|\vec{p}_2''\vec{k}_{31}''\rangle\langle\vec{p}_2''\vec{k}_{31}''|V_2|\vec{p}_1'\vec{k}_{23}\rangle}{S-p_2''^2/2\mu_2-k_{31}''^2/2\mu_{31}}, \quad (2.19)$$

where the Green's function was defined in Eq. (2.3). Using Eqs. (2.7), (2.8), and (2.11) the matrix element of V_2 becomes

$$\langle\vec{p}_2''\vec{k}_{31}''|V_2|\vec{p}_1'\vec{k}_{23}\rangle=\langle\vec{p}_2''\vec{k}_{31}''|V_2|\vec{p}_2'''\vec{k}_{31}'''\rangle$$
$$=\frac{Z_1Z_3e^2\delta(\vec{p}_2''-\vec{p}_2''')}{2\pi^2|\vec{k}_{31}''-\vec{k}_{31}'''|^2}, \quad (2.20)$$

where

$$\vec{p}_2'''=-(\mu_{23}/m_3)\vec{p}_1'-\vec{k}_{23},$$
$$\vec{k}_{31}'''=(\mu_{31}/\mu_1)\vec{p}_1'-(\mu_{31}/m_3)\vec{k}_{23}.$$

Similarly evaluating the matrix element for V_1 and utilizing the two δ functions, Eq. (2.19) can be written

$$\langle\vec{p}_2'\vec{k}_{31}|V_1G_0V_2|\vec{p}_1'\vec{k}_{23}\rangle=\frac{Z_1Z_2Z_3^2e^4}{4\pi^4}\frac{1}{|\vec{k}_{23}+\vec{B}|^2}$$
$$\times\frac{1}{|\vec{k}_{31}-\vec{A}|^2}\left[S-\frac{1}{2\mu_2}\left(\frac{\mu_{23}}{m_3}\vec{p}_1'+\vec{k}_{23}\right)^2\right.$$
$$\left.-\frac{1}{2\mu_{31}}\left(\vec{k}_{31}-\frac{\mu_{31}}{m_3}\vec{k}_{23}-\frac{\mu_{31}}{m_3}\vec{B}\right)^2\right]^{-1}. \quad (2.21)$$

Equation (2.21) may now be inserted into Eq. (2.18). Finally, the change of variables $\vec{k}_1=\vec{k}_{23}+\vec{B}$ and $\vec{k}_2=\vec{k}_{31}-\vec{A}$ leaves Eq. (2.18) in the form

$$\langle\Phi_f^{(2)}|V_1G_0V_2|\Phi_i^{(1)}\rangle=\frac{-32\mu_{31}Z_1Z_2Z_3^2e^4\lambda^5}{\pi^3}$$
$$\times\int\frac{d\vec{k}_1}{k_1^2}\frac{I_{12}}{[\lambda^2+(\vec{k}_1-\vec{B})^2]^2}, \quad (2.22)$$

where

$$I_{12}\equiv\int\frac{d\vec{k}_2}{k_2^2}\frac{\{\lambda^2+(\vec{k}_1-\vec{B})^2+2\vec{k}_2\cdot[\vec{A}-(\mu_{31}/m_3)\vec{k}_1]+k_2^2\}^{-1}}{[\lambda^2+(\vec{k}_2+\vec{A})^2]^2}. \quad (2.23)$$

In a similar manner, the matrix elements of $V_1G_0V_3$ and $V_3G_0V_2$ can be reduced to this form. The results are

$$\langle\Phi_f^{(2)}|V_1G_0V_3|\Phi_i^{(1)}\rangle=\frac{-32\mu_{23}Z_1Z_2^2Z_3e^4\lambda^5}{\pi^3}$$
$$\times\int\frac{d\vec{k}_1}{k_1^2}\frac{I_{13}}{[\lambda^2+(\vec{k}_1+\vec{A})^2]^2}, \quad (2.24)$$

where

$$I_{13}\equiv\int\frac{d\vec{k}_2}{k_2^2}\frac{[-2\mu_{23}S+(\vec{k}_1+\vec{A})^2+(\mu_{23}/\mu_2)p_2'^2-2\mu_{23}\vec{k}_2\cdot(\vec{k}_1/m_3+\vec{B}/\mu_{23})+k_2^2]^{-1}}{[\lambda^2+(\vec{k}_2-\vec{k}_1-\vec{B})^2]^2}, \quad (2.25)$$

$$\langle\Phi_f^{(2)}|V_3G_0V_2|\Phi_i^{(1)}\rangle=\frac{-32\mu_{31}Z_1^2Z_2Z_3e^4\lambda^5}{\pi^3}\int\frac{d\vec{k}_1}{k_1^2}\frac{I_{32}}{[\lambda^2+(\vec{k}_1+\vec{B})^2]^2}, \quad (2.26)$$

where

$$I_{32}\equiv\int\frac{d\vec{k}_2}{k_2^2}\frac{[-2\mu_{31}S+(\vec{k}_1+\vec{B})^2+(\mu_{31}/\mu_1)p_1'^2+2\mu_{31}\vec{k}_2\cdot(\vec{k}_1/m_3+\vec{A}/\mu_{31})+k_2^2]^{-1}}{[\lambda^2+(\vec{k}_2+\vec{k}_1+\vec{A})^2]^2}. \quad (2.27)$$

The three integrals I_{12}, I_{13}, and I_{32} are all of the same form and can be done analytically. The details are given in the Appendix. This reduces three of the second-order Born terms to a single vector integral.

The last second-order term is $V_3G_0V_3$ which contains the proton-proton interaction twice. For this term, the analog of Eq. (2.19) is

$$\langle \vec{p}_2' \vec{k}_{31} | V_3 G_0 V_3 | \vec{p}_1' \vec{k}_{23} \rangle = \int d\vec{p}_3 \int d\vec{k}_{12} \times \frac{\langle \vec{p}_2' \vec{k}_{31} | V_3 | \vec{p}_3 \vec{k}_{12} \rangle \langle \vec{p}_3 \vec{k}_{12} | V_3 | \vec{p}_1' \vec{k}_{23} \rangle}{S - p_3^2/2\mu_3 - k_{12}^2/2\mu_{12}} \quad . \quad (2.28)$$

The δ functions derived from evaluating the two potentials in Eq. (2.28) make it more convenient to eliminate the variables $\vec{k}_{31}$ and $\vec{k}_{23}$ in terms of the set $\vec{p}_3$ and $\vec{k}_{12}$ in the complete matrix element, Eq. (2.9). Then, the change of variables

$$\vec{k}_1 = \frac{\mu_{12}}{m_1} \vec{p}_3 - \vec{k}_{12} + \vec{p}_2' \quad \text{and} \quad \vec{k}_2 = \vec{p}_3 + \vec{p}_1' + \vec{p}_2'$$

leads to

$$\langle \Phi_f^{(2)} | V_3 G_0 V_3 | \Phi_i^{(1)} \rangle = \frac{-32\mu_{12} Z_1^2 Z_2^2 e^4 \lambda^5}{\pi^3} \times \int d\vec{k}_2 \frac{I_{33}}{[\lambda^2 + (\vec{k}_2 - \vec{A})^2]^2 [\lambda^2 + (\vec{k}_2 - \vec{B})^2]^2} \quad , \quad (2.29)$$

where

$$I_{33} \equiv \int \frac{d\vec{k}_1}{k_1^2} \left[\frac{\mu_{12}}{\mu_{31}} [\lambda^2 + (\vec{k}_2 - \vec{A})^2] + 2\mu_{12} \vec{k}_1 \cdot \left(\frac{\vec{p}_1'}{m_1} - \frac{\vec{p}_2'}{m_2} - \frac{\vec{k}_2}{m_1} \right) + k_1^2 \right]^{-1} \Big/ (\vec{k}_1 - \vec{k}_2)^2 \quad . \quad (2.30)$$

I_{33} is of a slightly different form than Eq. (2.23). It is evaluated analytically in the Appendix.

This completes the demonstration that the second-order Born terms can be analytically reduced from six-dimensional to three-dimensional integrals. No approximations were made concerning the relative masses of the three particles. However, as a convenience to the proton-hydrogen problem, $m_1 = m_2$ was freely used. In Sec. III some numerical results are presented.

III. NUMERICAL RESULTS

The three-dimensional integrals representing the second-order Born terms, Eqs. (2.22), (2.24), (2.26), and (2.29) were evaluated numerically for several energies from 0.1 to 2.5 MeV. In Table I the cross sections calculated in the various approximations discussed in Sec. I are compared. In this energy region, backward scattering is completely negligible and the Jackson–Schiff cross section represents the correct first-order Born approximation. Above 0.5 MeV, the exact second-order cross section is smaller than the other approximations.

Drisko's high-energy formula for the second-order cross section is[10]

$$\sigma_D = (5\pi v/2^{12} + 0.295)\sigma_{BK} \quad , \quad (3.1)$$

where v is the velocity of the incident proton and σ_{BK} is given in Eq. (2.14). The first term in Eq. (3.1) is about 10% of the second term at 2 MeV. Several of the results of Drisko's high-energy analysis are violated in the energy region considered here. His results show that the terms $V_1G_0V_3$ and $V_3G_0V_2$ have negligible imaginary parts, and that the sum of these two terms exactly cancels the first-order term V_3. Together with his demonstration that $V_3G_0V_3$ is smaller than all the other first- and second-order terms at high energy, these considerations show that the proton-proton interaction V_3 is unimportant in calculating the rearrangement cross section to second order for forward-scattering angles. However, in the exact calculation, the imaginary parts of all the second-order terms are important, frequently being larger (by order of magnitude in some cases) than the real parts. The over-all sign of the real parts of the terms $V_1G_0V_3$ and $V_3G_0V_2$ varies as a function of the scattering angle. With increasing energy the real parts of these terms become increasingly negative as is required to cancel the positive term V_3. Finally, the doubly repulsive term $V_3G_0V_3$ is of the same order of magnitude as the other second-order terms in this energy region although its role slowly decreases with increasing energy.

In Fig. 1, the cross sections given in Table I are shown as a function of E^{-6} for E units of 100

TABLE I. Proton-hydrogen electron-transfer total cross sections in atomic units. The approximations are those used by Brinkman–Kramers (Ref. 4) (BK), Jackson-Schiff (Ref. 6) (JS), Drisko (Ref. 10) (D), and the present calculation (II).

E (MeV)	Cross sections in a.u. BK	JS	D	II
0.1	1.26	0.231	0.381	0.360
0.5	1.03×10^{-3}	3.16×10^{-4}	3.22×10^{-4}	2.96×10^{-4}
1.0	2.50×10^{-5}	9.23×10^{-6}	7.98×10^{-6}	6.58×10^{-6}
1.5	2.56×10^{-6}	1.04×10^{-6}	8.31×10^{-7}	6.74×10^{-7}
2.0	4.92×10^{-7}	2.12×10^{-7}	1.62×10^{-7}	1.43×10^{-7}
2.5	1.35×10^{-7}	6.09×10^{-8}	4.50×10^{-8}	4.20×10^{-8}

keV. Asymptotically, $\sigma_{BK}E^{+6}$ approaches 40.2 [Eq. (2.14)], while $\sigma_{JS}E^{+6}$ approaches 0.661 of this value. Drisko's result is still approximating an E^{-6} behavior, since the first term in Eq. (3.1) has not yet dominated the second. At very much higher energies (~100 MeV), Eq. (3.1) will begin to display an $E^{-5.5}$ behavior and at still larger energies (~1000 MeV) σ_D will become greater than σ_{BK}. However, at these energies backward scattering invalidates Eq. (3.1). At higher energies than those considered here (say, 10–50 MeV), the exact second-order calculation should follow σ_D through its region of validity and then display the dominant E^{-3} behavior of the correct first-order cross section.

An additional feature of adding in the second-order terms is shown in Fig. 2. The first-order differential cross section of Jackson and Schiff dips to zero at some small scattering angle which is slightly energy dependent. This is due to cancellation between the matrix elements of V_1 and V_3 which are always of opposite sign. The tail of the first-order differential cross section contributes from 5% to 10% of the total cross section. The complete second-order differential cross section is monotonic in behavior and decreases more rapidly at larger scattering angles than the first-order curve.

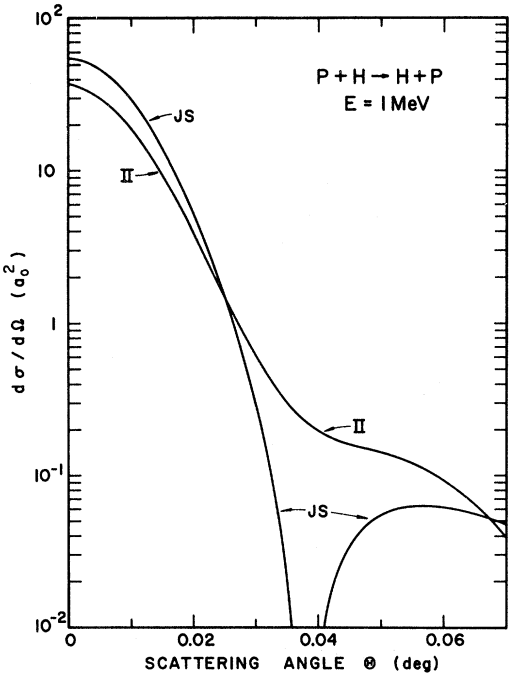

FIG. 2. Proton-hydrogen electron-transfer differential cross section in atomic units as a function of the center-of-mass scattering angle in degrees. The lab energy is 1 MeV. The approximations are described in Table I.

IV. CONCLUSIONS

The basic question of the role of the proton-proton interaction in the Born series for proton-hydrogen electron-transfer collisions has been settled at very high energies by the dominant role of the first-order repulsive term V_3. At intermediate energies, such as those considered here, all of the first- and second-order terms are important. In fact, the higher-order terms may well play a significant role.[10] However, if these terms contribute an energy dependence no greater than E^{-6}, then Drisko's cross section could be useful at energies up to an order of magnitude higher than the energies investigated here.

A useful test of the various approximations would be comparison with experiment. Unfortunately, the various experiments[14] are not always in good agreement and extend up to only 100 or 200 keV. It is necessary to include the effects of capture into excited states when making a comparison with experiment. Finally, the calculation of the cross section in the higher MeV ranges requires the addition of relativistic effects.

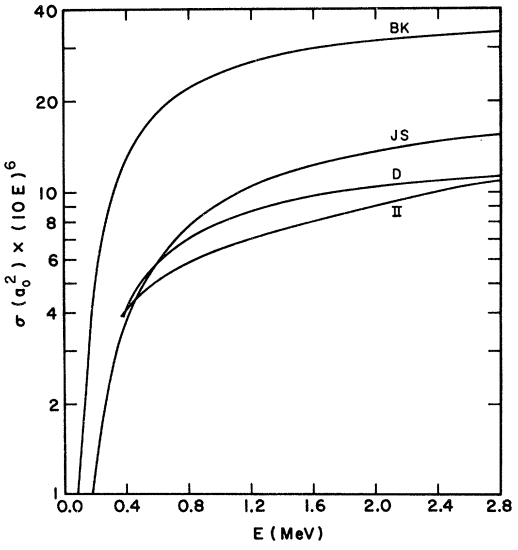

FIG. 1. Proton-hydrogen electron-transfer total cross section in atomic units multiplied by $(10E)^6$ for E in MeV as a function of energy. The various approximations are described in Table I.

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APPENDIX

The integrals I_{12}, I_{13}, I_{32} are each of the form

$$I=\int \frac{d\vec{W}}{W^2}\,\frac{1}{(X_1+2\vec{W}\cdot\vec{V}_1+W^2)^2}\cdot\frac{1}{(X_2+2\vec{W}\cdot\vec{V}_2+W^2)}\ , \tag{A1}$$

where X_1, X_2, $\vec{V}_1$, and $\vec{V}_2$ are independent of W. Using the Feynman integral formula[15]

$$\frac{1}{a^2 b} = 2\int_0^1 dX \frac{X}{[aX + b(1-X)]^3} . \tag{A2}$$

Equation (A1) becomes

$$I = 4\pi \int_0^1 dX\, X \int_0^\infty dW \int_{-1}^1 dz\, (W^2 + 2WV_3 z + X_3)^{-3} , \tag{A3}$$

where

$$\vec{V}_3 = X\vec{V}_1 + (1-X)\vec{V}_2 \quad \text{and} \quad X_3 = X_1 X + (1-X)X_2 . \tag{A4}$$

The integrals over W and z can be done in a straightforward manner to give

$$I = \frac{\pi^2}{2}\int_0^1 dX \frac{X(3X_3 - 2V_3^2)}{X_3^2 (X_3 - V_3^2)^{3/2}} . \tag{A5}$$

The transformation $y = X(X_1 - X_2) + X_2$ changes Eq. (A5) to

$$I = \frac{\pi^2}{2} \frac{1}{(X_1 - X_2)^2} \int_{X_2}^{X_1} dy \frac{\alpha_1 y^3 + \alpha_2 y^2 + \alpha_3 y + \alpha_4}{y^2 (\alpha_5 y^2 + \alpha_6 y + \alpha_7)^{3/2}} , \tag{A6}$$

where

$$\alpha_1 = -2(\vec{V}_1 - \vec{V}_2)^2/(X_1 - X_2)^2 ,$$

$$\alpha_2 = 3 + 2[(2X_1 + X_2)V_2^2 + 3X_2 V_1^2 - 2(X_1 + 2X_2)\vec{V}_1 \cdot \vec{V}_2]/(X_1 - X_2)^2 ,$$

$$\alpha_3 = -2V_2^2 - 3X_2 - 2X_2[3X_2 V_1^2 + (4X_1 - X_2)V_2^2 - (4X_1 + 2X_2)\vec{V}_1 \cdot \vec{V}_2]/(X_1 - X_2)^2 ,$$

$$\alpha_4 = 2X_2 (X_1 \vec{V}_2 - X_2 \vec{V}_1)^2/(X_1 - X_2)^2 ,$$

$$\alpha_5 = \tfrac{1}{2}\alpha_1 ,$$

$$\alpha_6 = 1 + 2[X_1 V_2^2 + X_2 V_1^2 - (X_1 + X_2)\vec{V} \cdot \vec{V}_2]/(X_1 - X_2)^2 ,$$

$$\alpha_7 = -\alpha_4/2X_2 . \tag{A7}$$

Defining

$$J_n = \int dy \frac{1}{y^n (\alpha_5 y^2 + \alpha_6 y + \alpha_7)^{3/2}} , \tag{A8}$$

the final result can be expressed as

$$I = \frac{\pi^2}{2} \frac{1}{(X_1 - X_2)^2} (\alpha_1 J_{-1} + \alpha_2 J_0 + \alpha_3 J_1 + \alpha_4 J_2)_{y=X_2}^{y=X_1} . \tag{A9}$$

The integrals J_n can be done analytically.

The quantity $X_2 + 2\vec{W} \cdot \vec{V}_2 + W^2$ in Eq. (A1) actually represents the free-particle Green's function G_0. This can have a simple pole within the range of integration. However, the final result [Eq. (A9)] will automatically produce the correct imaginary part for the second-order Born terms.

The special cases $X_1 = X_2$ with or without $\vec{V}_1 = \vec{V}_2$ can occur and are best treated by returning to Eq. (A5) and then simplifying the expressions X_3 and $\vec{V}_3$ at that step.

The form of the integral I_{33} differs from Eq. (A1) only in that both factors in the denominator are raised to the first power. Use of the appropriate Feynman formula and the same transformation leads to a much simpler result

$$I_{33} = \frac{\pi^2}{(X_1 - X_2)} \frac{1}{(-\alpha_7)^{1/2}} \left[\sin^{-1}\left(\frac{\alpha_6 y + 2\alpha_7}{y(\alpha_6^2 - 4\alpha_5\alpha_7)^{1/2}} \right) \right]_{y=X_2}^{y=X_1} , \tag{A10}$$

where the α's were defined in Eq. (A7).

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